3.6   Overview of Computational Energy Sciences at NETL

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Abstract

NETL has initiated an in-house activity entitled Computational Energy Sciences to develop methods and tools for simulating fossil energy components and systems. The long term goal of this activity is to develop the ability to construct virtual simulations of future vision 21 processes and plants. These virtual plants would incorporate simulations and models of the major components of the plant, detailed simulations of critical sub-elements and processes, and overall simulations of process dynamics, performance, and economics. Currently, NETL is developing models of multiphase flow components, turbine combustors, fuel cells, gasifiers, and PC-fired boilers. Visualization of components and simple systems is also being initiated. NETL is working in close collaboration with several regional univeristies, the Pittsburgh Supercomputer Center, other national labs, and several industrial partners in this activity.

National Energy Technology Laboratory

Overview of Computational Energy Sciences at NETL

Jack Halow

November 07, 2001

Vision 21 Program Review Meeting

Onsite Science and Technology Research

- **Four Focus Areas** and two technology clusters

- Involves 1/3 of staff

- 31 CRADA's

- Research laboratories at Morgantown and Pittsburgh

Carbon Sequestration Science
Large stationary sources of CO_2

Ultra-Clean Fuels
For high-efficiency transportation systems

Gas Energy Systems Dynamics
Gaseous-fueled power generation systems

Computational Energy Science
Virtual demonstrations of energy plants of the future

Computational Energy Sciences Focus Area

- An NETL "in-house" collection of people, activities and resources established to develop modeling and simulation methods for fossil energy systems

- Partnerships with universities, national labs and industry basic to its structure

- Cross-cuts all of the fossil energy programs

Past Work and Present Investigations

Past Work

- **Gas-Solids MFIX code developed**

- **Extensive use of Fluent Code single phase flow**

- **Geological Modeling for Natural Gas production**

- **Extensive use of ASPEN code for systems Modeling**

- **Engineering models developed with experimental studies**

Present Investigations

- **Multiphase flow predictions**

- **Single phase flow using Fluent code**

- **Computational Chemistry**

- **Virtual Demonstration**

- **Dynamic process and control models**

- **New approaches to fast simulation in fossil energy**

Virtual Simulation

- ## Objectives
  - Develop models and simulations of key FE systems
  - Develop computing and visualization resources for FE
  - Expand personnel engaged in FE simulation

- ## Technical Challenges
  - Large variety of technologies must be addressed
  - Complexity of processes to be modeled

- ## Technical Approach
  - Extend current models to all fossil energy systems
  - Establish/develop key new computational methods
  - Aggressively form partnerships to develop these capabilities

We need models on different scales

- **Mesa-scale**
  - **Constitutive laws built upon fundamental science**
  - **Computational Chemistry**

- **Device scale**
  - **Mass, energy and momentum transfer relationships to predict unit performance**
  - **CFD as an example**

- **System scale**
  - **Includes engineering and control models**

  - **Simulations of coupled systems to understand large scale and complex interactions and to develop models for control**

Models we are now developing

- **Mesa-scale**
  - **Constitutive laws for multiphase flow**
  - **Computational chemistry of membranes and catalysts**

- **Device scale**
  - **Turbine combustors**
  - **Circulating fluidized beds**
  - **Transport gasifiers**
  - **PC fired boilers including biomass co fire**
  - **Hot gas particulate filters**
  - **Fuel cells**

- **System Scale**
  - **Dynamic Response of turbine fuel cell systems**
  - **CFB dynamic and control models**

MFIX MULTIPHASE CFD CODE

Past Development

- MFIX code -- general purpose multiphase hydrodynamics, heat transfer and chemical reactions

- Hydrodynamics:constitutive equations, bubbling, circulating and spouted beds

- Chemistry: coal combustion/gasification, FCC, desulfurization

- Applications: Foster Wheeler carbonizer, PyGas gasifier, bubbling fluid beds
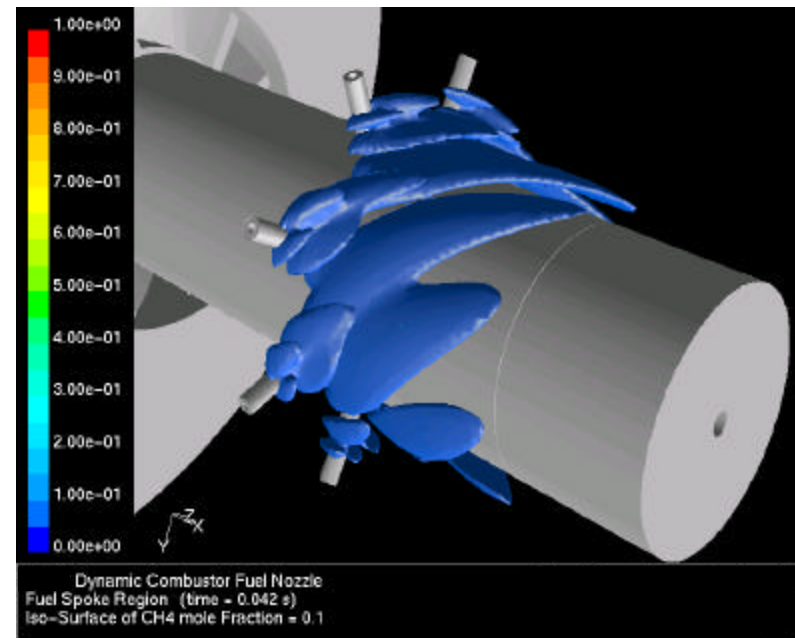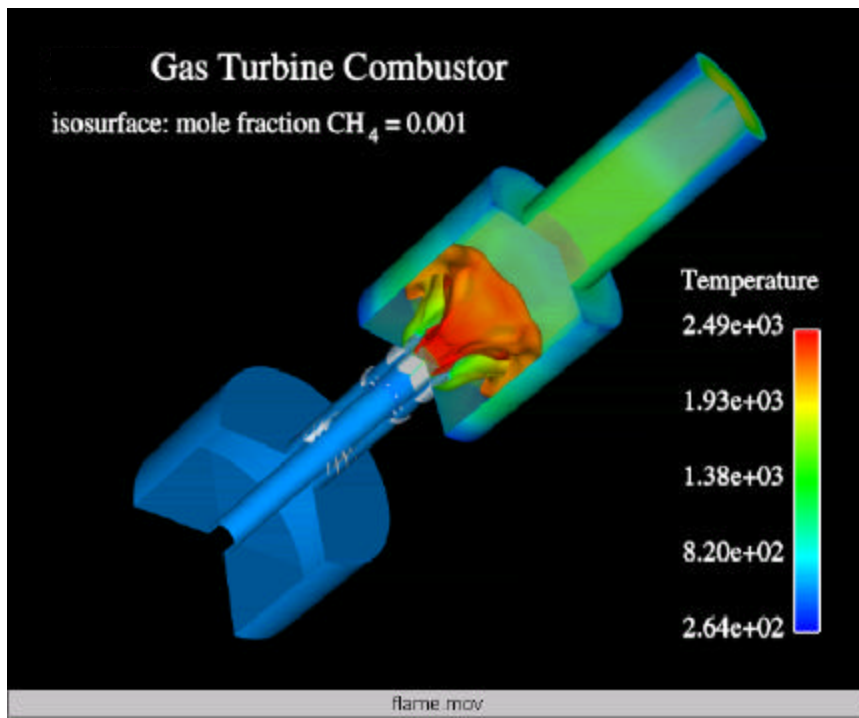
Current Activities

- OIT project/MFDRC

- Improving numerics: robust solution algorithms, higher order methods

- Adding chemistry: Ozone decomposition, silane pyrolysis, silicon hydrochlorination, methane combustion
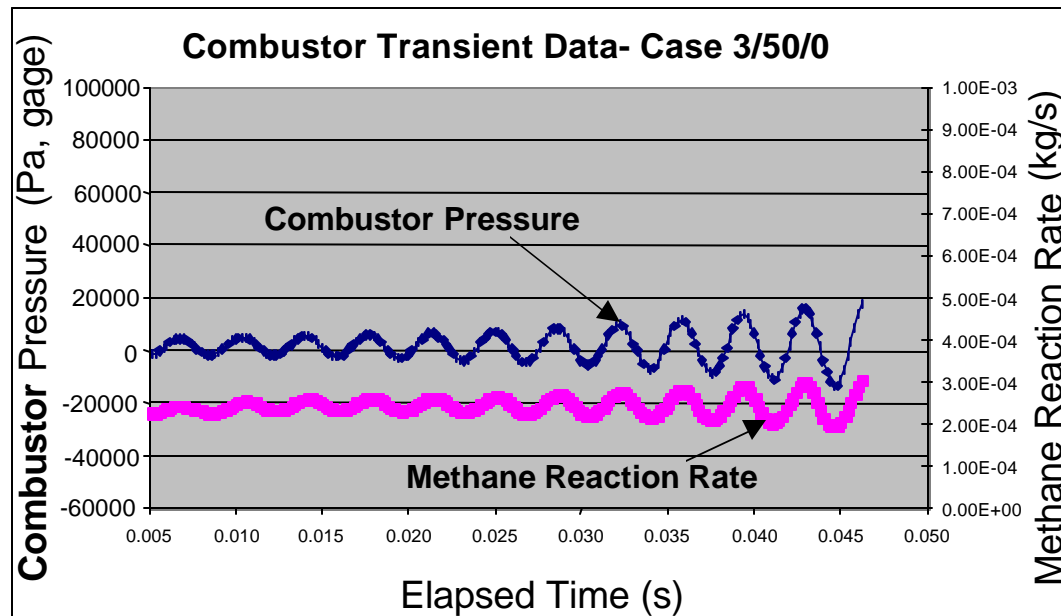
- Applications: Circulating fluidized beds

MFIX Simulation of Circulating Fluidized Bed
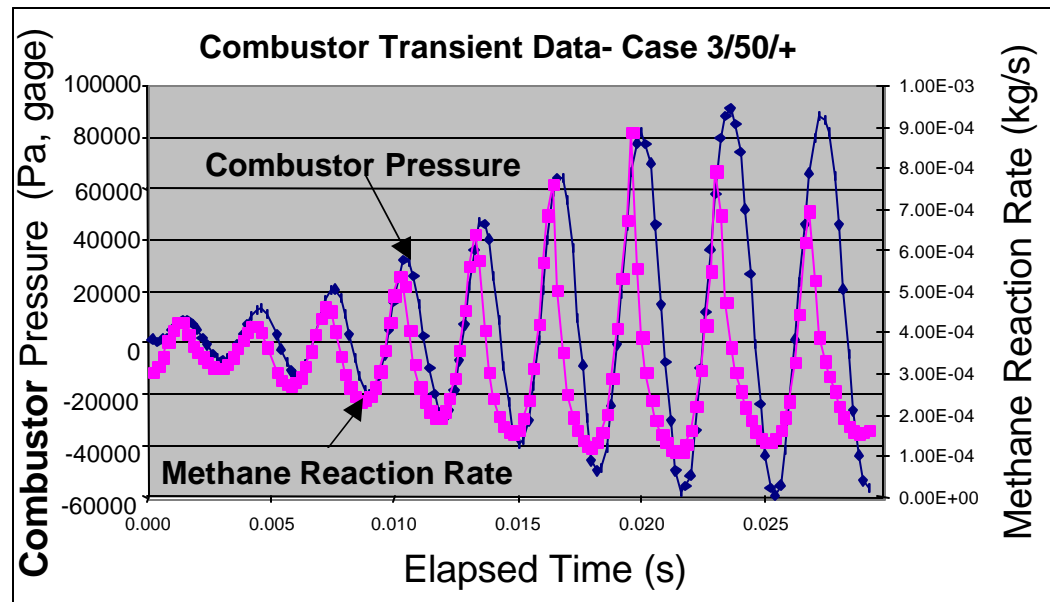
Turbine Combustor Simulations

Gas Turbine Combustor

isosurface: mole fraction CH$_4$ = 0.001

Temperature
2.49e+03
1.93e+03
1.38e+03
8.20e+02
2.64e+02

flame.mov

1.00e+00
9.00e-01
8.00e-01
7.00e-01
6.00e-01
5.00e-01
4.00e-01
3.00e-01
2.00e-01
1.00e-01
0.00e+00

Dynamic Combustor Fuel Nozzle
Fuel Spoke Region (time = 0.042 s)
Iso-Surface of CH4 mole Fraction = 0.1
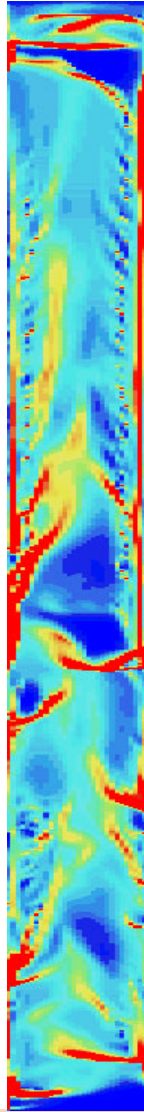
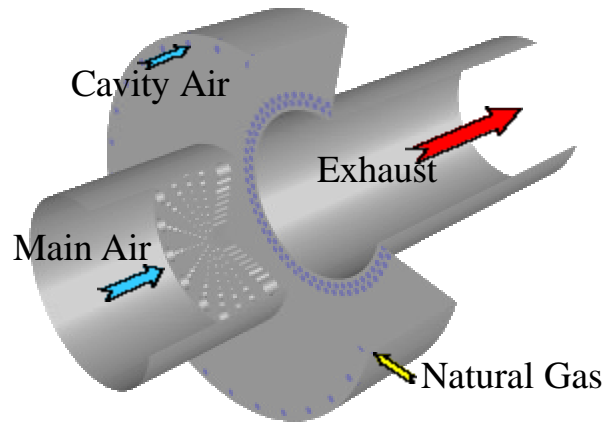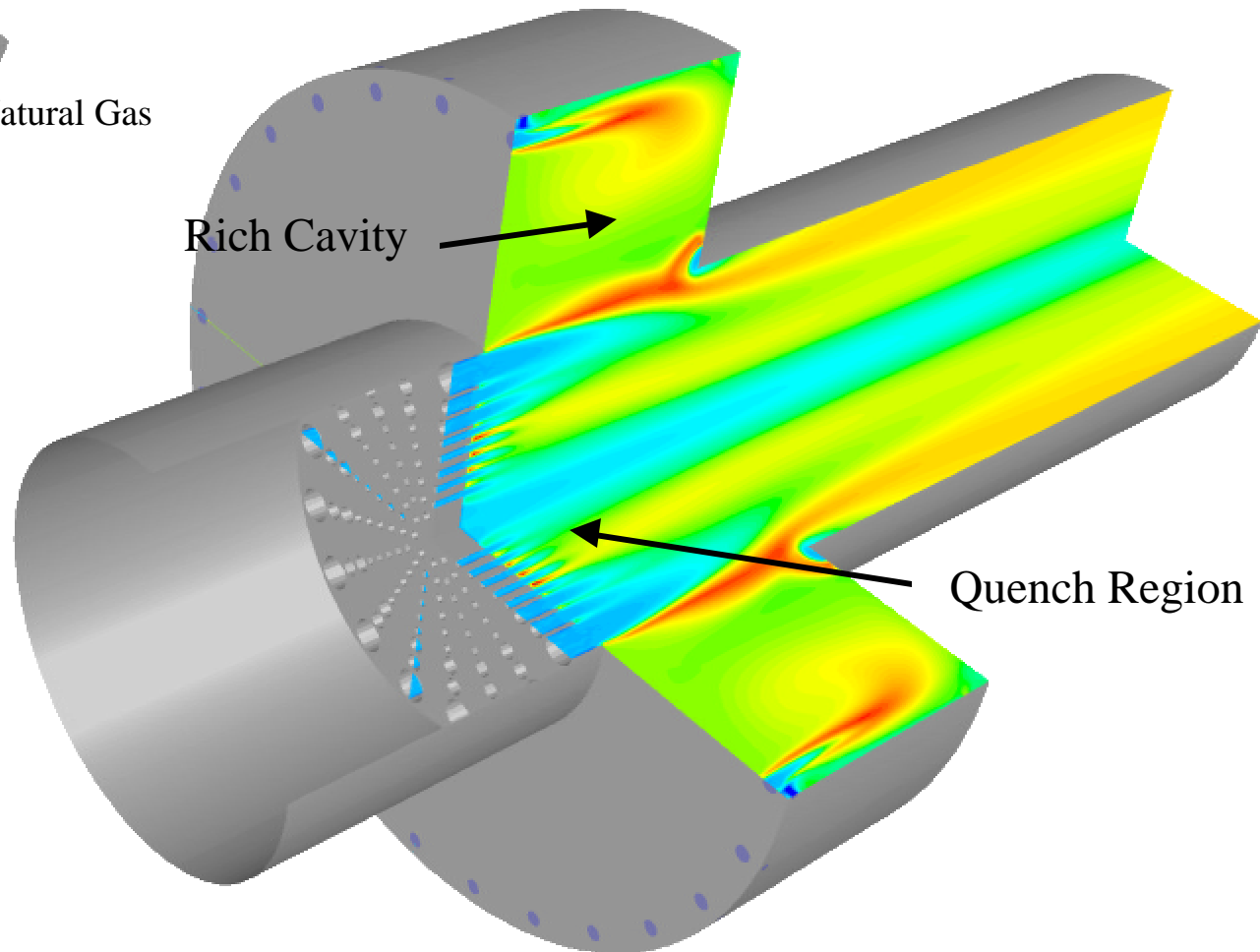# Combustor Simulations

Combustor Transient Data- Case 3/50/0

Stable: $\phi = 0.6$

Unstable: $\phi = 0.8$

TVC Combustor Simulations

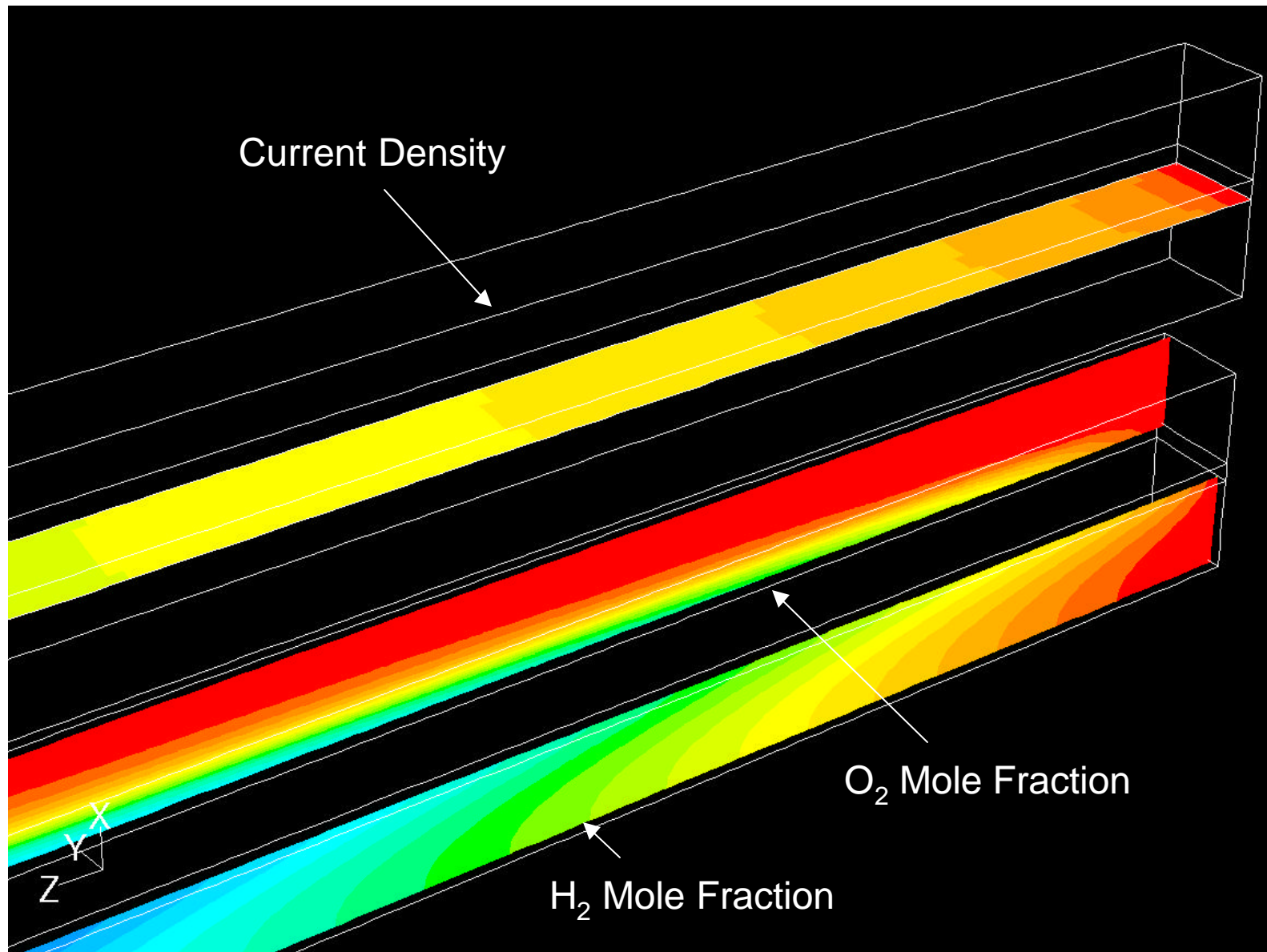Cavity Air

Exhaust

Main Air

Natural Gas

Temperature (K)

2.03e+03
1.88e+03
1.74e+03
1.60e+03
1.45e+03
1.31e+03
1.16e+03
1.02e+03
8.76e+02
7.32e+02
5.88e+02
4.44e+02
3.00e+02

Rich Cavity

Quench Region

NETL

SOFC Model Overview

Local species concentration
and temperature imply local
ideal voltage and losses

FLUENT CFD	Electrochemistry
Species, momentum, energy eqns.	Model — Nernst eqn., equipotential condition

Current distribution
implies species and heat
fluxes at electrodes

Current Density

O₂ Mole Fraction

H₂ Mole Fraction
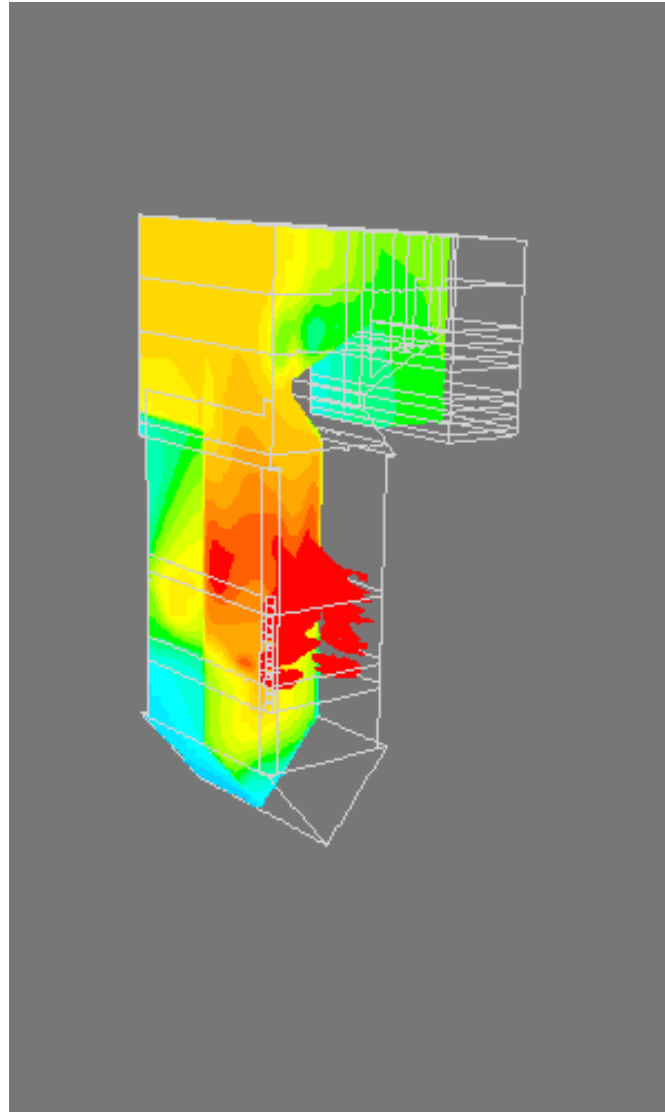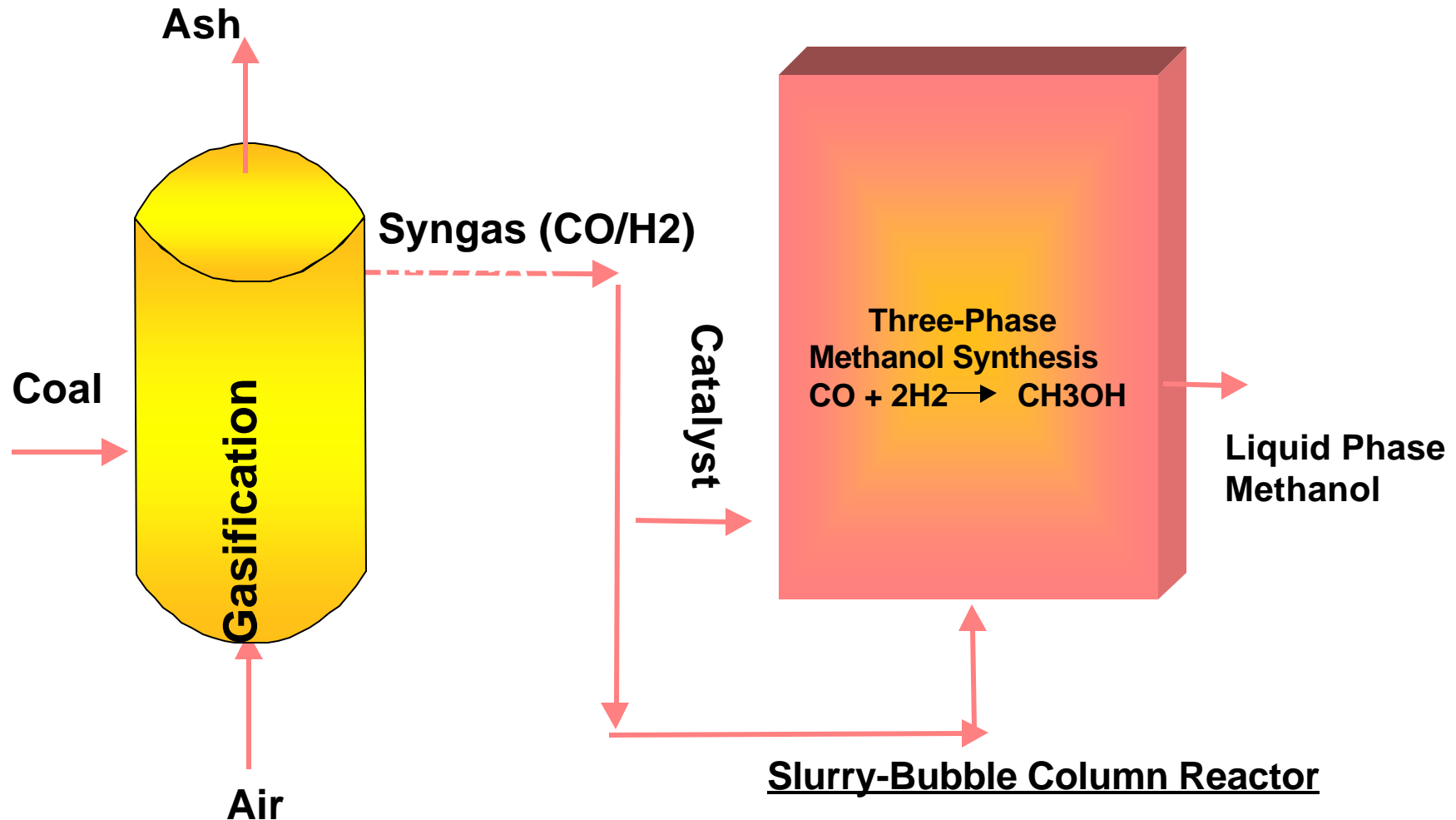
Fluent Simulation of flame in a PC Fired Boiler

Liquid fuels production
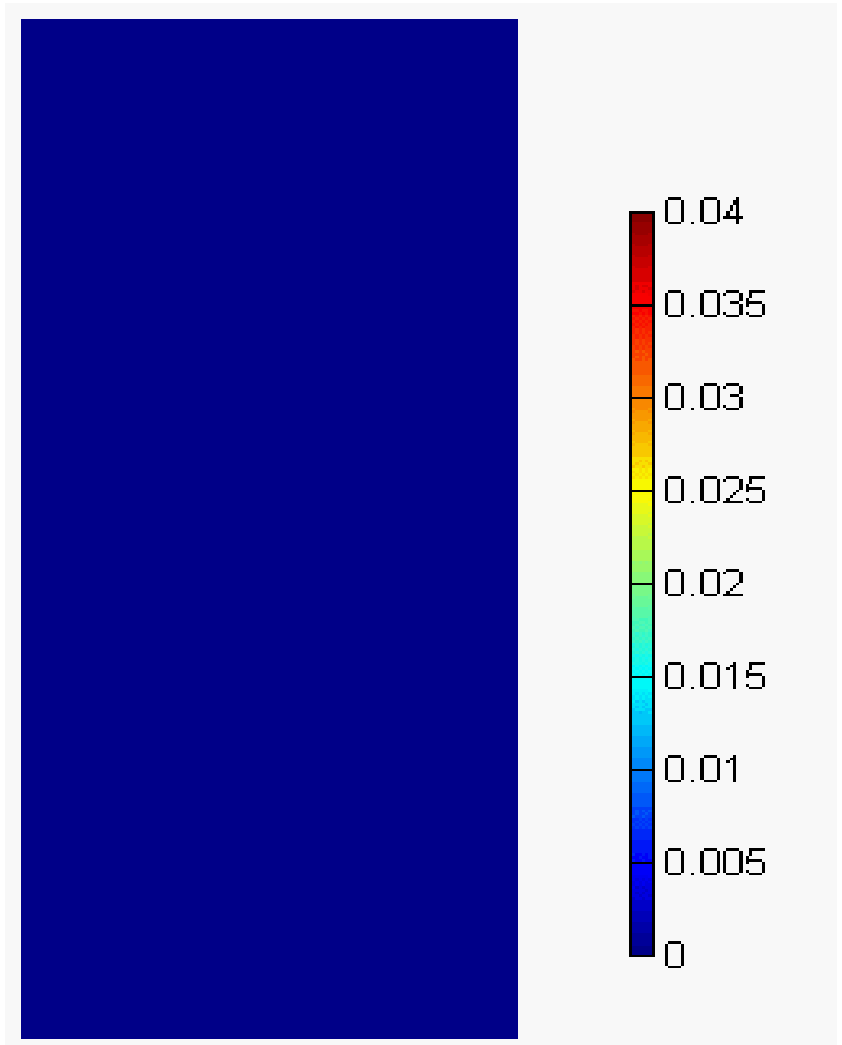
Simplified Diagram of Conversion of Coal into Methanol

Ash

Coal

Air

Gasification

Syngas (CO/H2)

Catalyst

Three-Phase
Methanol Synthesis
$CO + 2H_2 \longrightarrow CH_3OH$

Liquid Phase
Methanol

Slurry-Bubble Column Reactor

NETL

Predicted Methanol Mole Fraction

Configuration "A"
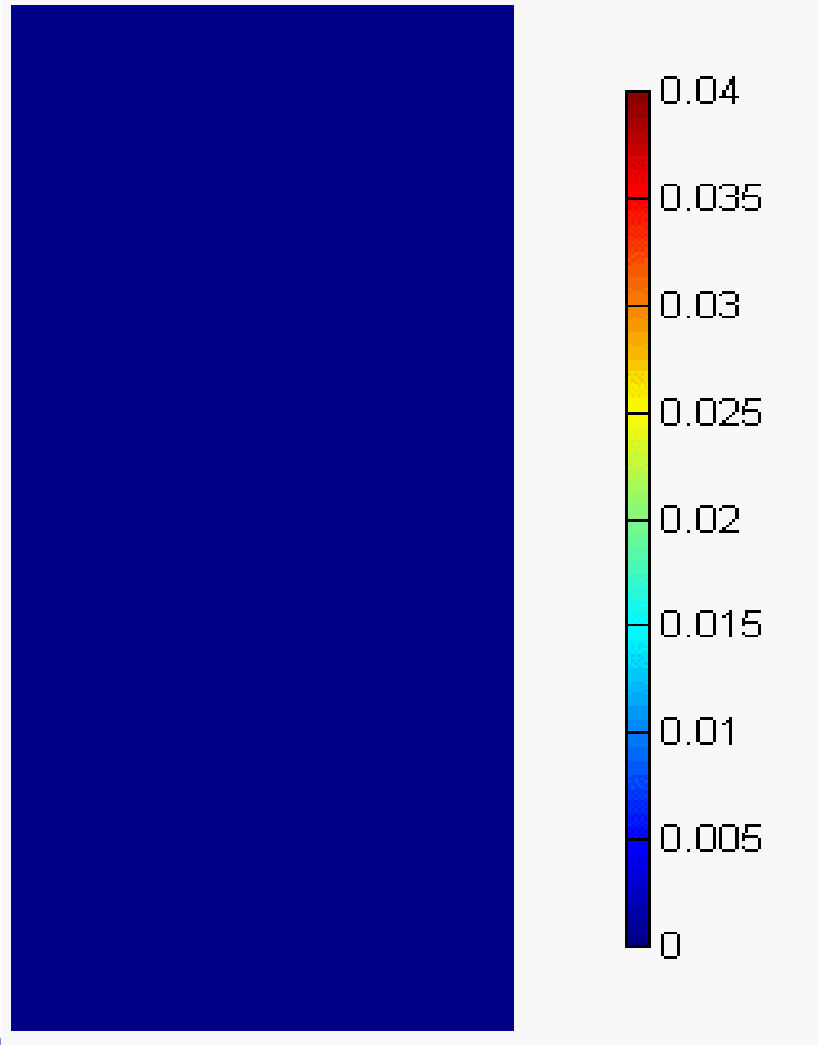
Configuration "B"

Transport Gasifier Model

- **Overall Objectives**

  - To validate the gasification model with experimental data provided by University of North Dakota Energy Environmental Research Center (UNDEERC)

  - To support Power Systems Development Facility (PSDF) gasification program

- **Technical Challenges**

  - Inclusion of gasification chemistry in FLUENT

  - Addition of light gas pyrolysis product composition

Predicted Vs. measured species

Product gas	Volume fraction (predicted)	Volume fraction (experiment)
CH4	2.33 %	6.7 %
CO	8.61 %	12.7 %
CO2	24.15 %	28.3 %
H2	21.78 %	20.7 %
N2	43.13 %	31.6 %

|	simulation	experiment
Temperature at the outlet (F)	1702	1650
Velocity in the riser (ft/s)	44.5	44.2
Carbon conversion	60.81 %	62.4* %

*   gas make

Computational Chemistry to Examine Hydrogen Storage Potential

-Much current interest in carbon nanotubes for H2 storage

-DOE target for H_2 storage is 6.5 wt%

-Sample purification & characterization greatly complicate experiments

-Molecular simulations using carefully calibrated potentials allow prediction of H_2 physisorption as function of T, P, tube size, tube packing,….

0.6 wt%
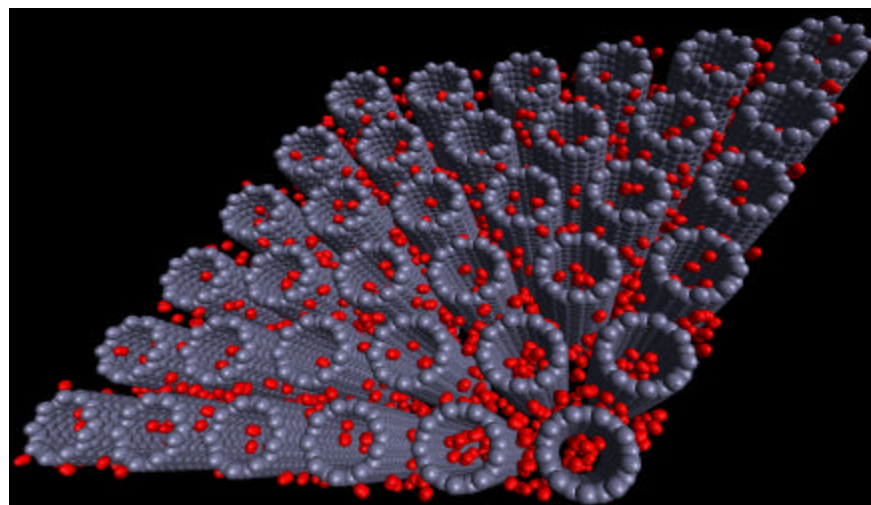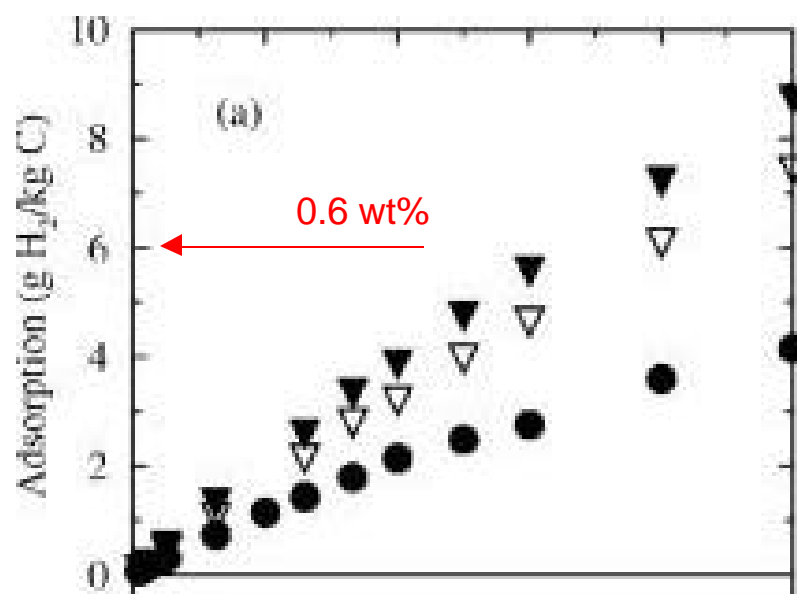
Real Cold Flow Circulating Fluidized Bed

Low Order and Novel Models

• Pressure balance model predicts one dimensional pressure balance and flow Regimes

• Dynamic Neural Network Model evaluates control options

• Kalman Filter Analysis for real-time control

• Emergent Behavior Bubble Model predicts bubble dynamics and conversion in dense bed regions

• Smooth Sphere Hydrodynamics provides a way to rapidly calculate complex single phase flows.

Emergent Behavior Model of Fluidized Bed
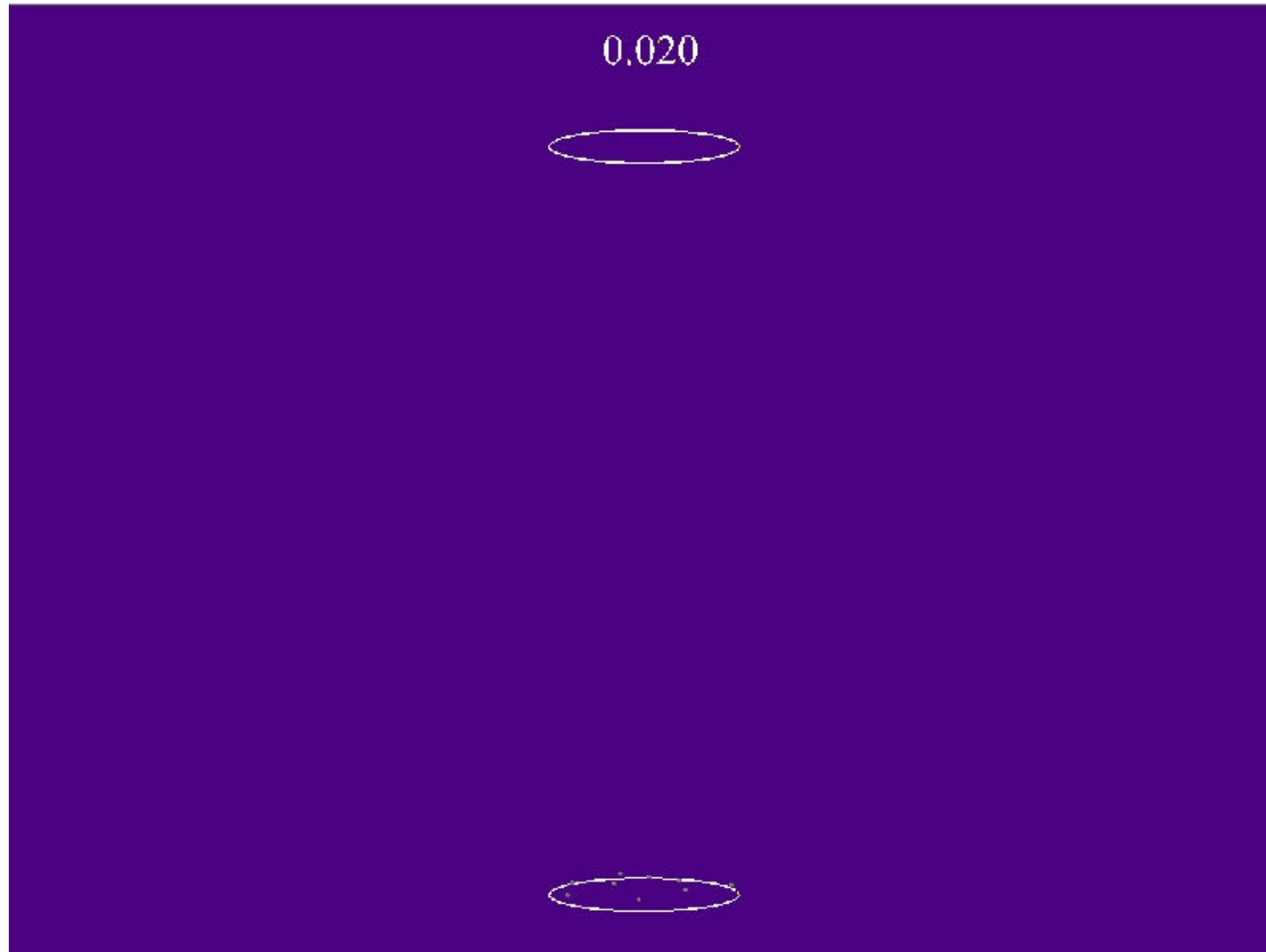
Visualization

- **The power of visualization is its ability to convey meaning.**

- **Almost half of the human brain is used to process visual information. We are inherently "visual creatures"**

- **In science, context comes from numbers and formulas as well as words. Numbers and formulas are best expressed as visual information.**

- **If a picture is worth a thousand words, a visual simulation is worth a million numbers**

NETL Virtual Environments Lab

- **Purpose is to develop virtual representations of FE projects, site, and facilities and to incorporate models and simulations into these virtual plants**

- **Partnership formed with WVU Virtual Environments Center**

- **Facility established**

- **NETL onsite virtual projects(3) developed**

Virtual NETL Distributed Power Project
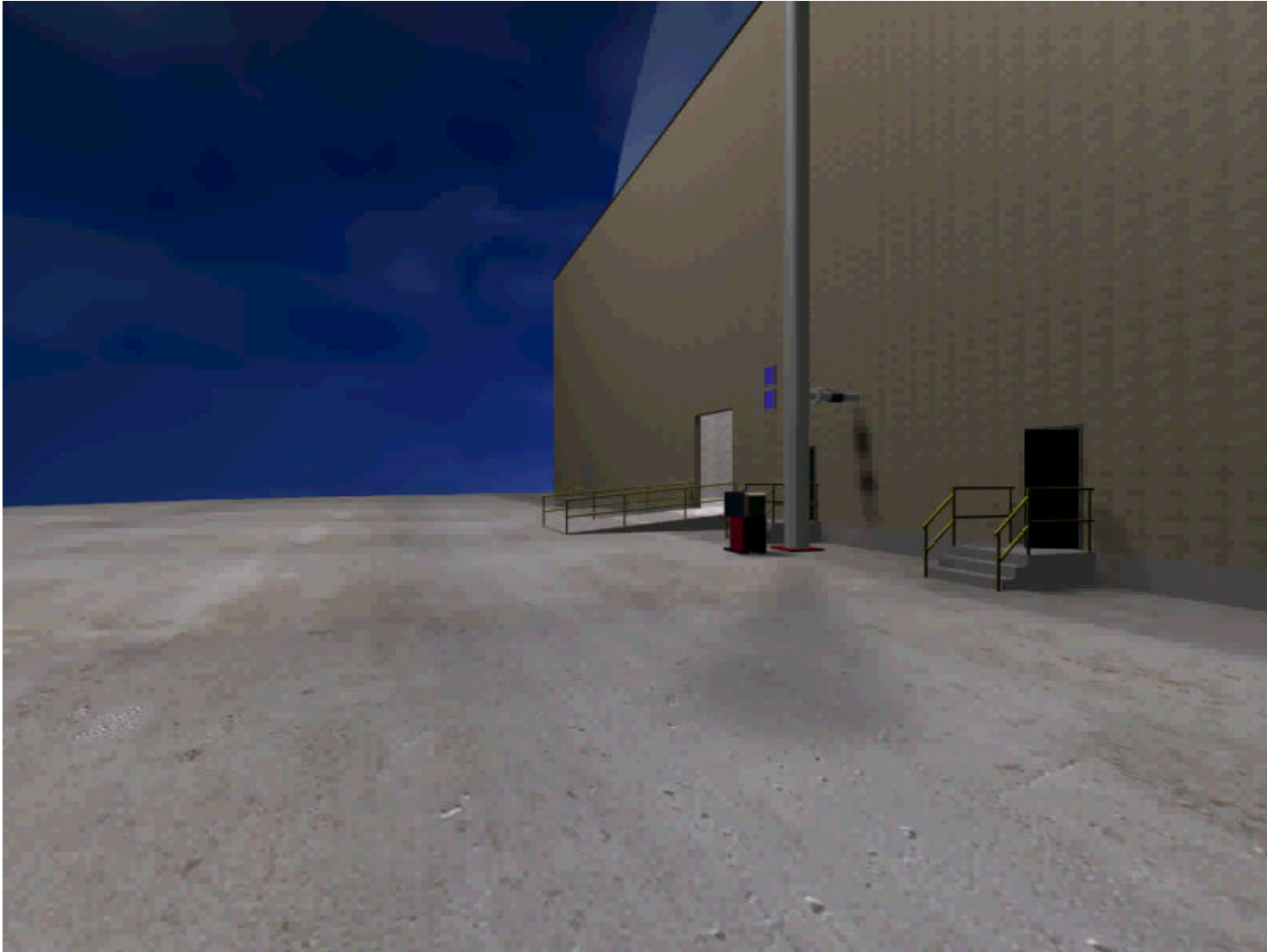
Virtual Cold Flow Circulation Fluidized Bed
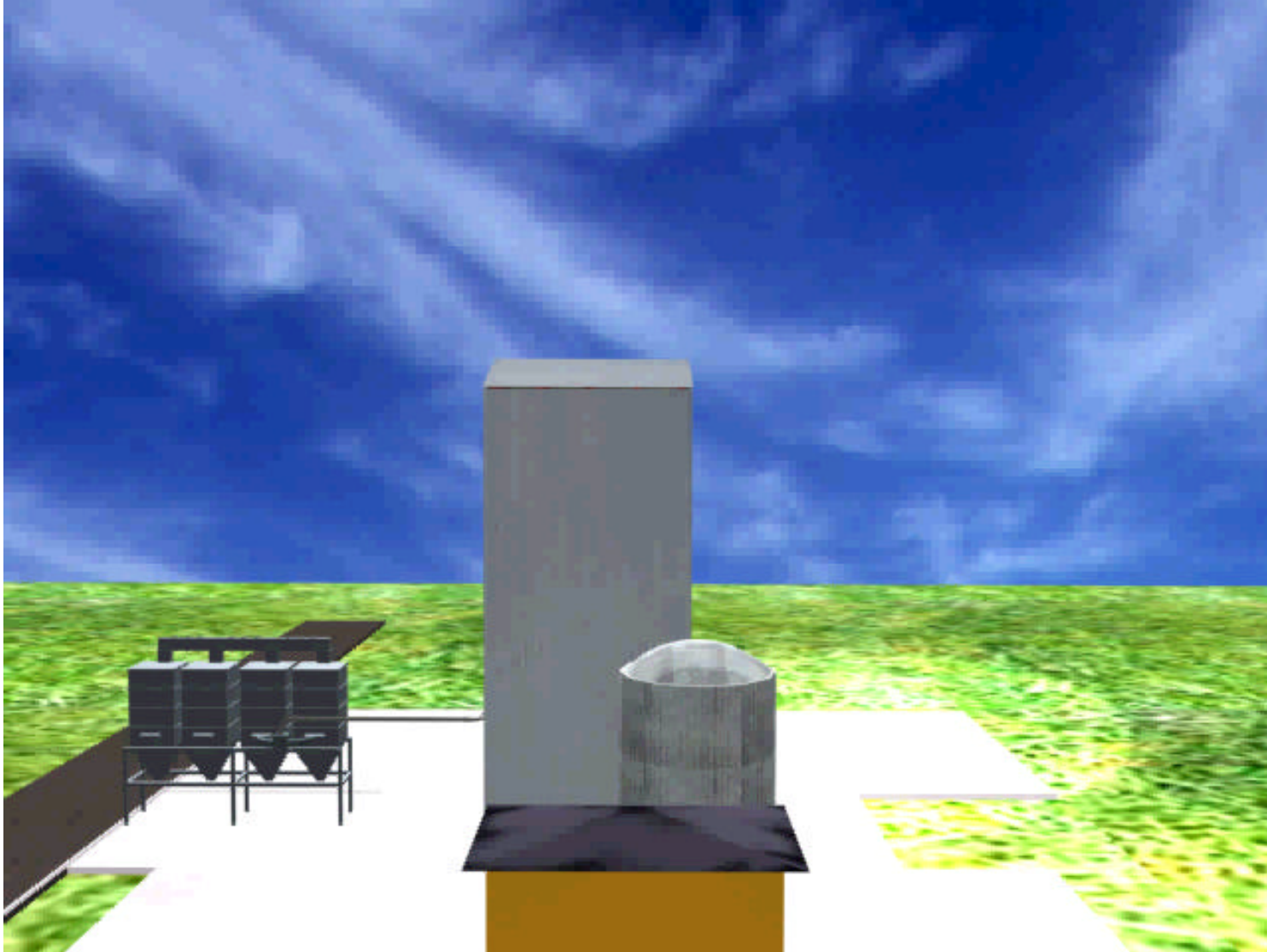
Partnerships

- **Universities: WVU, CMU, Pitt, Princeton. IIT, UT, PSU, PSC, Iowa State, Clarkson,Texas A&M, Auburn**

- **Industry: Foster Wheeler, Fluent, Aeolus, Dow Corning, ABB, Westinghouse**

- **Other Government: ORNL, SNL,PNNL, LANL, EE/OIT, NASA**

- **SC^2: Regional Consortium for scientific supercomputing-- NETL, PSC, WVU, CMU, Pitt, State of West Virginia, Duquesne U, Penn State**

Plans

- **Plans for the Next 12 Months**
  - Complete B-3 Virtual environments facility
  - Acquire codes additional FE devices
  - Create library of virtual fossil plant components

- **Longer Term Plans**
  - Port simulations and models into virtual environments
  - Simulate complete new Vision 21 plants

Computer Improvement

1982

- In 1982, a 10mb IBM hard drive cost $3000 or $300/mb
- The IBM PC ran at a clock speed of 86 kHz
- Memory was 128k
- Mass storage was 256 kilobytes on a 5 1/2 inch floppy was SOA

2001

- 20 gb hard drive can be bought for $60 or 3 cents/mb
- PCs runs at 1.7 gigahz
- Memory of 1 or 2 gbyte
- Mass storage of terabyte(s) is easy to obtain

Computing changing how we solve problems

- **Transition from slide rules to laptops is a revolutionary change**
  - Time for calculations greatly shorten
  - Accuracy greatly improved
  - Approach can be different: with a slide rule, experimentation was the exploratory phase and calculation was the final step.
  - Now calculation can be exploratory with numeric experiments or simulations based on good models.
  - Experimentation can be the final step to confirm the simulation

Some predictions about the future

"From a semiconductor manufacturing perspective, there is no limit to the ability of our industry to increase density, performance and integration for the next 20 years, sure it gets more expensive to build fabs but the price per function will still reduce faster than the cost per unit area, and at a geometric rate.

Tim Chambers – STMicroelectronics VP and GM

More Predictions about the future

About embedded computers: …."Already, a modern automobile has far more computing power than the craft we landed on the moon. …. We will live in a ubiquitous, all-seeing, all-hearing network, that will envelope all but the most remote parts of the planet."

Ben Delaney – CyberEdge, President

More Predictions about the future

I lump communication with computing because the value of a computer is much more in its presentation ability than in its computational strength. It does no good to calculate faster if you cannot communicate the results of those calculations quickly and comprehensibly. Already most people use there computers as a communications device.

Ben Delaney – CyberEdge, President

Virtual Future Ultra-Clean Coal Power Plant
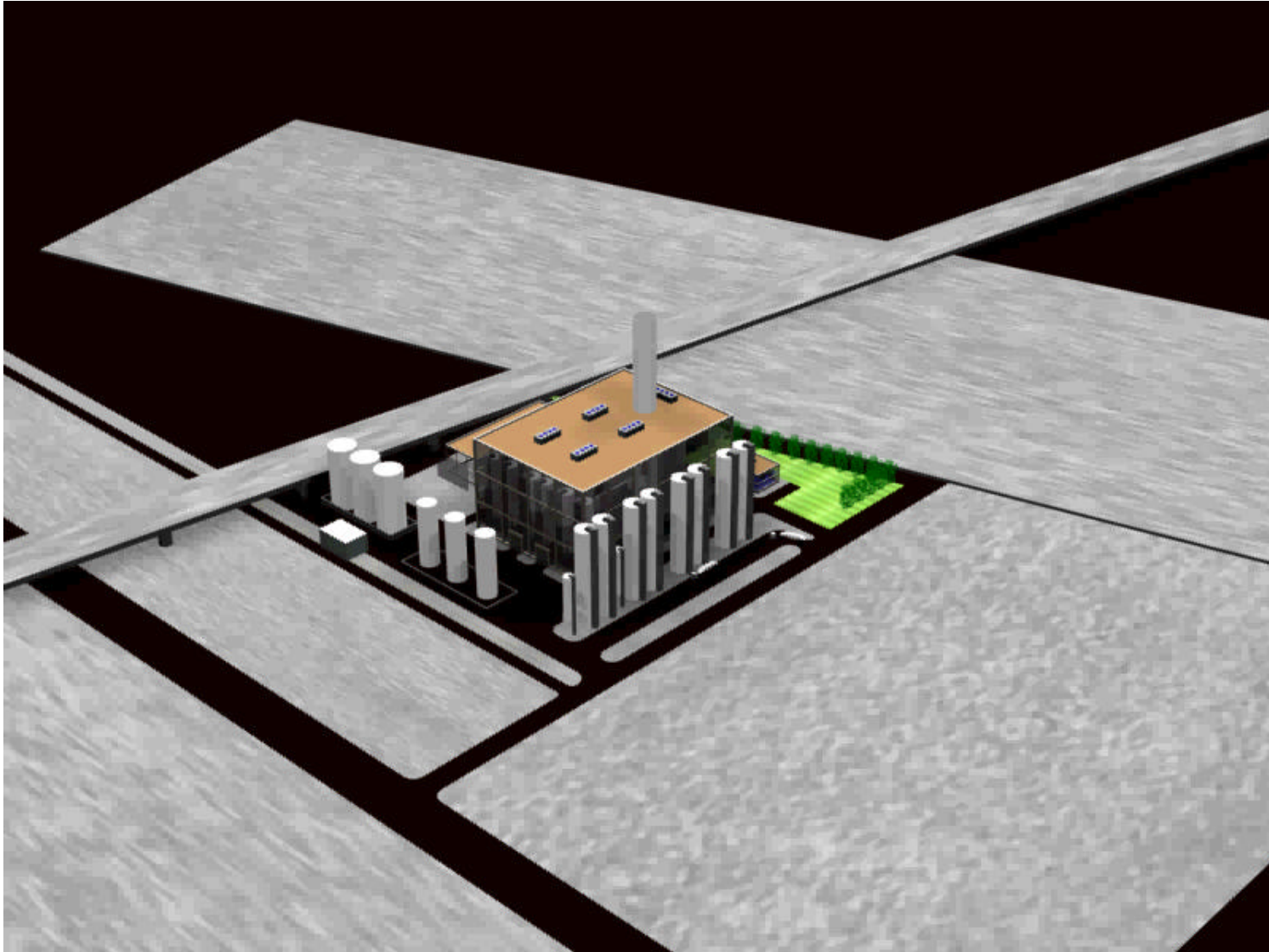
Computational Resources

- 29 high end PC's (450, 500 & 933 1,700 mhz)

- Three Beowulf clusters: 24, 72, & 128 processors (a fourth is under construction) at Morgantown Site

- 20 Processor Beowulf at Pittsburgh Site

- Older SGI machines

- The Pittsburgh Supercomputing Center (PSC) with Cray T3E, Intel quad processor cluster and new quad processor alpha cluster under construction

- Fluent, MFIX, Matlab, Protrax, Aspenplus, Intergraph Smart Plant Review, Mathematica, Ensight, Irix, Visual Basic, Fortran, C++, Paragon, Java, 3D Studio Max, Pro E, Adobe Premier, Tech Plot, AVS, Opendx, other software

Cluster Methodology

- **Basic Building Blocks:**
  - Commodity PC hardware
  - Commodity networking equipment
  - Linux operating system
- **Implementation Requirements:**
  - Modifications to basic OS and hardware configurations to match parallel application requirements. (Often requires unique approaches.)
  - Modifications to the operating system kernel and device drivers to optimize system performance.
  - Careful maintenance to assure system-wide stability.

Visualization Resources

- **Computational Energy Sciences Center**
  - 10 high end 3D NT workstations
  - Four Emersive workstations
  - One 3-sided "CAVE" (WVU through SC^2)
  - Large screen conference room
  - 100Mb Ethernet
- **Uses:**
  - **Simulation & Modeling**
  - **Graphics Rendering**
  - **Virtual Environments for NETL**
  - **Visitors**

Scientific LAN

- **High Speed Scientific LAN will link B2 Beowulf clusters, B-3 Visualization Labs, B-26 & T45 scientific workstations.**

- **OC3 line will connect to Pittsburgh Supercomputer Center and through PSC Gigapop to High speed networks**

- **SciLan provides both secure and open connections**

- **Pittsburgh site can access Morgantown resources through gigapop**

(SC)^2 Partnership

- **Regional consortium to promote supercomputing and high speed connectivity**

- **Members: WVU, CMU, Pitt, PSC, Penn State, other regional colleges, State of West Virginia**

- **Gives NETL access to the PSC supercomputers and gigapop**

Predictions about the future

Reality Blur: …."Simulations will astound us and virtual worlds, if not totally interactive, will become a major part of our lives—in many cases without us even being aware of it….a new psychosis will develop called reality blur where we get confused between what we experience via media and what is happening in real life."

Jon Peddie, consultant